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High Resolution Electron Energy Loss Spectroscopy Studies of Chemisorbed Species on Metal Surfaces

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

The objective of this research program is to utilize high resolution electron energy loss spectroscopy and other spectroscopic tools to investigate chemical and physical properties of surfaces and of gas-surface interactions. Our experiments address issues pertaining to bond lengths and site symmetry of chemisorbed atoms and molecules at metal surfaces, binding energies and vibrational frequencies associated with the atomic and molecular bonds, and with the driving mechanisms responsible for structural transformations which occur at surfaces as a result of chemisorption or other perturbations such as temperature change. Our work also addresses possible improvements in experimental techniques and data analysis which offer expanded applications.

Research accomplishments of the program include a significant advancement in instrumentation, the first measurements of shear horizontal vibrational modes at crystal surfaces, the first detection of projected bulk phonon modes by surface electron scattering and elucidation of novel properties associated with hydrogen interaction at Nb surfaces.

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19 The first observation of shear horizontal modes on Ni(100), Ag(100) and Ag(110) was made possible by the capability of our new instrument to detect out-of-plane scattering, combined with the improved sensitivity of the electron optics. Our new results including the shear modes constitute the first complete characterization of all surface vibrational modes at a single crystal surface. These data provide tests of selection rules that govern inelastic electron scattering and are presently being used in conjunction with lattice dynamical calculations to refine our understanding of interatomic potentials that bind crystals and govern thin film growth, and interface stability.

Inelastic electron scattering and angle resolved photoemission studies of the interaction of H with Nb have established the existence of a metastable subsurface binding site of hydrogen just below the surface. The location of the hydrogen site (tetrahedral) has been deduced based on vibrational data, and the novel thermal properties of the site occupation have been studied by photoemission and electron scattering. These studies have provided a detailed microscopic basis for explaining the novel uptake kinetics associated with the H/Nb system and have tested calculations of the ground state electronic properties of Nb and the H/Nb system.

FINAL REPORT

AFOSR-86-0109

This Final Report summarizes significant accomplishments and research progress achieved during the past three and one-half years (1 April 1986 - 31 October 1989) under a grant from the Chemical and Atmospheric Sciences Division of AFOSR (Grant #AFOSR-86-0109).

The objective of this research program is to utilize high resolution electron energy loss spectroscopy and other spectroscopic tools to investigate chemical and physical properties of surfaces and of gas-surface interactions. Our experiments address issues pertaining to bond lengths and site symmetry of chemisorbed atoms and molecules at metal surfaces, binding energies and vibrational frequencies associated with the atomic and molecular bonds, and with the driving mechanisms responsible for structural transformations which occur at surfaces as a result of chemisorption or other perturbations such as temperature change. Our work also addresses improvements in experimental techniques and data analysis which offer expanded applications of inelastic electron scattering spectroscopy.

The attachment to this write-up contains data covering FY costs, inclusive dates, personnel, and a complete list of publications and technical presentations covering the grant period is presented at the end of the write-up. Significant accomplishments are grouped into subsections with appropriate reference to the resulting publications.

New Instrumentation for Inelastic Electron Scattering

One of the most important fundamental objectives of surface science is to characterize the atomic-level forces that govern chemisorption, thin film nucleation and growth, and surface/interface properties including (for example) surface reconstruction and interface stability. The most sensitive and effective experimental probe of these atomic-level forces is through a combination of surface phonon measurements and lattice dynamical analysis.

Our group, under AFOSR sponsorship, has made a significant advancement in experimental techniques required to probe surface phonons by inelastic electron scattering. We have advanced the state-of-the-art in inelastic electron scattering instrumentation in two important areas. First, we have constructed a new instrument capable of studying inelastic scattering using out-of-plane scattering geometry. This innovation now permits detection of odd-symmetry shear modes which are very sensitive to details of the surface interction potentials, especially in the surface plane. In-plane interactions are particularly important in strained epitaxial layers and in surface reconstruction. The second advancement is a technical achievement in improving electron analyzer performance by incorporating multichannel electron energy detection. While this innovation has been available for several years in ESCA instruments, and has also been successfully applied to EELS instruments in applications requiring only moderate (10 meV) energy resolution, our instrument achieves 4 meV energy resolution at the high energies (several hundred eV incident energy) required for surface phonon spectroscopy.

Our design concept, including additional novel features such as tandem four-element zoom lens systems, was presented[3] in 1986, shortly after our analysis of the image properties of hemispherical analyzers (F. Hadjarab and J.L. Erskine, *J. Electron Spectr. Rel. Phenom.* **36**, 227 (1985)), had established the feasibility of high-resolution multichannel detection. Subsequent publications have reported ray tracing analysis of the four-element zoom lenses[13], including some new results for the properties of four-element lenses, and the vastly improved performance that was achieved by our new instrument[11]. Preliminary results from the new instrument including the first detection of odd-symmetry shear modes at metal surfaces are now being presented at scientific meetings and are being prepared for publication.

We have recently begun to explore the consequences of including odd-symmetry shear modes in the lattice dynamical analysis of surface phonon properties. In our initial studies of Ag(100) surfaces, we have found that knowledge of these modes dramatically affects the interaction potential models derived from phonon structure. (An abstract is attached which has been submitted to the Vibrations at Surfaces Conference IV.) Our new results indicate that many of the conclusions, arrived at based on models that consider only even symmetry modes, should be reconsidered with the addition of shear mode properties.

Hydrogen Adsorption on W(100)

We carried out a series of studies[6,9] including lattice dynamical analysis of β_1H on W(100) in which a new hydrogen derived vibrational mode was discovered and explained. The new mode turned out to be an optical mode arising from inter-atomic coupling between adjacent hydrogen atoms (there are two H atoms per unit cell for the saturated coverage phase). Our lattice dynamical analysis of this system yielded an estimate of the coupling potential associated with the H-H interactions (it turned out to be approximately 1/10 of the H-W interaction). In addition, these studies revealed a new resonance scattering mechanism which occurs when certain kinematical conditions are used in the experiment, namely conditions under which diffracted electron beams begin to emerge from the surface.

Hydrogen Interactions at Nb Surfaces

We carried out a series of experiments which investigated the novel properties associated with the up-take of hydrogen by Niobium. Our first experiments[4] based on inelastic electron scattering established the interesting fact that hydrogen adsorbs at sites just below the surface, and that the site exhibits a novel reversible temperature dependence. In subsequent experiments[8,10] using angle-resolved photoemission, we studied the bulk and surface electronic properties of Nb and tested the predictions of first-principles calculations for bulk and surface electronic properties. We also verified the novel subsurface adsorption behavior associated with hydrogen up-take suggested by our earlier electron scattering studies. Our photoemission results also established a new technique for probing the spatial extent of near-surface electron states based on the way in which local electromagnetic fields affect the photoelectron cross-section for "s" and "p" polarized light.

Nitrogen Adsorption on W(100)

Nitrogen adsorption on W(110) provides a particularly interesting system for fundamental studies in surface science because both atomic and molecular chemisorption occurs depending on the surface temperature and dose. We carried out several studies[12] of this system using inelastic electron scattering which established several new vibrational modes, and which resulted in reassignment of some previously discovered modes. Our experiments also discovered and explored a new ordered chemisorbed phase of N_2 on W(100).

Review Article

A comprehensive review[7] of the field of inelastic electron scattering was prepared for and published by CRC Press.

A. Refereed Journals:

1. J. L. Erskine, "High-Resolution Electron Energy Loss Spectroscopy: Explored Regions and the Frontier", *J. Vac. Sci. Technol.A* **4**, 1282 (1986).

2. J. P. Woods and J. L. Erskine, "Surface Vibrational Resonances and the Order-disorder Transformation at the W(100) Surface", *J. Vac. Sci. Technol.A* **4**, 1414 (1986).

3. J. L. Erskine, "Advanced Electron Optics for Vibrational Spectroscopy", *J. Electron Spectroscopy Rel. Phenom.* **39**, 265 (1986).

4. Ying Li, J. L. Erskine, and A. Diebold, "High Resolution Electron Energy Loss Spectroscopy of Hydrogen Chemisorption at Nb(100) Surfaces: Evidence for Subsurface Adsorption Sites", *Phys. Rev.B* **34**, 5951 (1986).

5. J. P. Woods and J. L. Erskine, "High-Resolution Low-energy Electron Reflection from W(100) Using the Electron Energy Loss Spectrometer: A Step Towards Quantitative Analysis of Surface Vibrational Spectra", *J. Vac. Sci. Technol.* **4**, 435 (1987).

6. J. P. Woods, A. D. Kulkarni, J. L. Erskine, and F. W. deWette, "Vibrational Properties of β_1H and β_1D on W(001): Electron Energy Loss Measurements and Lattice-dynamical Calculations", *Phys. Rev.B* **36**, 5848 (1987).

7. J. L. Erskine, "High Resolution Electron Energy Loss Spectroscopy", *CRC Critical Reviews*, CRC Press **13**, (4), 311 (1987).

8. Bo-Shung Fang, C. A. Ballentine, and J. L. Erskine, "Electronic Properties of Nb and H Treated Nb Surfaces", *Phys. Rev.B* **36**, 7360 (1987) (*Rapid Communications*).

9. J.L. Erskine, J.P. Woods, A.D. Kulkarni, and F.W. deWette, "Surface Vibrations on Clean and Hydrogen Saturated W(100)", *J. of Electron Spectro. and Related Phenom.* **44**, 27 (1987).

10. B.-S. Fang, C.A. Ballentine, and J.L. Erskine, "Hydrogen Adsorption at Nb(100): Photoemission Evidence of Two-state Exchange Involving Subsurface States", *Surface Science Letters* **204**, L713 (1988).

11. Eue-Jin Jeong and J.L. Erskine, "Multichannel Detection High Resolution Electron Energy Loss Spectrometer", *Rev. of Scien. Instrum.* **60**, 3139 (1989).

12. A. Sellidj and J.L. Erskine, "Electron Energy Loss Spectroscopy Studies of Nitrogen Adsorption on W(100)", *Surface Science* **220**, 253 (1989).

13. A. Sellidj and J.L. Erskine, "A Tandem Four-element Lens System for Inelastic Electron Scattering Studies", *Rev. Sci. Inst.* **61** (1) 49 (1990).

14. J.L. Erskine, Eue-Jin Jeong, Joan Yater, Y. Chen, and S.Y. Tong, "Detection of Odd Symmetry Shear Modes at Metal Surfaces by Inelastic Electron Scattering: Experiment and Theory", (submitted to *J. Vac. Sci. and Tech.*,) (1989).

B. Invited Talks and Seminars

15. "Hydrogen Interactions at Niobium and Niobium Based Alloy Surfaces", J. L. Erskine, Symposium of the American Chemical Soc., Denver, Colorado, June 8-12, 1986.

16. "Electron Energy Loss Studies of Chemisorbed Underlayers at Metal Surfaces", J. L. Erskine, Department of Chemistry, University of Wisconsin, Madison, Wisconsin, Oct. 23, 1986.

17. "High Resolution Low Energy Electron Diffraction Studies of W Using an Electron Energy Loss Spectrometer", J. P. Woods and J. L. Erskine, 33rd National Symposium of the American Vacuum Society, Boston, Massachusetts, Oct. 27-31, 1986

18. "High Resolution Electron Energy Loss Spectroscopy Studies of the Interaction of H with Nb(100)", Y. Li, J. L. Erskine and A. Diebold, *Bull. Am. Phys. Soc.* **31**, 272 (1986)

19. "High Resolution Electron Energy Loss Spectroscopy of Adsorbates at Metal Surfaces", J. L. Erskine, Joint Meeting of the Texas Section of the APS and AAPT; Abilene Christian University, Abilene, Texas, March 6-7, 1987.

20. "Experimental Studies of the Interaction of H with Nb Surfaces" ,J. L. Erskine, 1987 Metal Hydrides Gordon Research Conference, Tilton School, Tilton, N.H., July 13-17, 1987.

21. "Surface Vibrations on Clean and Hydrogen Saturated W(100)", J.L. Erskine, J.P. Woods, A.D. Kulkarni, and F.W. deWette, Vibrations at Surfaces V, Eibsee Hotel, D-8104 Grainau-Eibsee, Fed. Rep. Germany, Sept. 6-10, 1987.

22. "Vibrational Spectroscopy Studies of Hydrogen at Metal Surfaces", J.L. Erskine, AFOSR Surface Chemistry Contractors Conference; Air Force Academy, Colorado Springs, Colorado, Sept. 16-18, 1987.

23. "Surface Vibrations on Clean and Hydrogen Covered Nb(110) Surfaces", Y. Li, A.D. Kulkarni, J.L. Erskine, and F.W. DeWette, March Meeting of the American Physical Society, New Orleans, Louisiana, March 21-25, 1988, *Bull. Am. Phys. Soc.* **33**, 655 (1988).

24. "Electron Energy Loss Spectroscopy Study of N_2 and H_2 Chemisorption on W(100) at 105K", A. Sellidj and J.L. Erskine, March Meeting of the American Physical Society, New Orleans, Louisiana, March 21-25, 1988, *Bull. Am. Phys. Soc.* **33**, 818 (1988).

25. "New Instrumentation Development: Multichannel Detection EELS", J.L. Erskine, AFOSR Molecular Dynamics Contractors Conference, Newport Beach, CA, Oct. 31 - Nov. 2, 1988.

26. "Multichannel Detection High Resolution Electron Energy Loss Spectrometer", Eue-Jin Jeong and J.L. Erskine, March Meeting of the American Physical Society, St. Louis, Missouri, March 20-24, 1989, *Bull. Am. Phys. Soc.* 34 (3) [1989].

27. "UPS Study of Nitrogen Adsorption on W(100) at 135 K", A. Sellidj and J.L. Erskine, March Meeting of the American Physical Society, St. Louis, Missouri, March 20-24, 1989, *Bull. Am. Phys. Soc.* 34 (3) [1989].

30. "Inelastic Electron Scattering Studies of Surface Phonons", J.L. Erskine, Department of Physics, Indiana University, Bloomington, Indiana, April 7, 1989.

31. "Detection of Odd-Symmetry Shear Modes at Metal Surfaces by Inelastic Electron Scattering: Experiment and Theory", J.L. Erskine, 36th National Symposium of the American Vacuum Society, Boston, Massachusetts, October 24-26, 1989.

32. "International Workshop on Surface Dynamics", Physics Department, University of Texas at Austin, Austin, Texas, November 9 - 11, 1989.

33. "Inelastic Electron Scattering from Surfaces and Thin Epitaxial Layers", J.L. Erskine, Molecular Dynamics Workshop, Captive Island, Florida, Oct. 29-31, 1989.

34. "Detection of Odd-symmetry Shear Modes at Metal Surfaces by Inelastic Electron Scattering: Experiment and Theory", J.L. Erskine, Eue-Jin Jeong, Joan Yater, Y. Chen, and S.Y. Tong, 36th National Symposium of The American Vacuum Society, Boston, Massachusetts, Oct. 23-27, 1989.

ATTACHMENT

COMPLETED PROJECT SUMMARY DATA

1.	TITLE	High Resolution Electron Energy Loss Spectroscopy Studies of Chemisorbed Species on Metal Surfaces.	
2.	PRINCIPAL INVESTIGATOR	J. L. Erskine Physics Department University of Texas Austin, Texas 78712	
3.	INCLUSIVE DATES	1 April 1986 - 31 Oct. 1989	
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6.	SENIOR RESEARCH PERSONNEL	None	
7.	JUNIOR RESEARCH PERSONNEL	J. Woods	(Ph.D. 1986)
		A. Sellidj	(Ph.D. 1989)
		E. Jeong	(Ph.D. 1989)
		Y. Li	(Ph.D. 1990)
		J. Yater	Student
8.	PUBLICATIONS		

SURFACE PHONONS OF Ag(100) AND Ag(110): THE IMPORTANCE OF ODD-SYMMETRY SHEAR MODES IN SEEKING ACCURATE INTERACTION MODELS

J.E. Yater, A.D. Kulkarni, F.W. deWette, and J.L. Erskine
Department of Physics
University of Texas
Austin, Texas 78712

Inelastic electron scattering measurements and lattice dynamical analysis of the vibrational properties of Ag(100) and Ag(110) surfaces are presented. The measurements include detection of odd-symmetry shear modes, and the lattice dynamical analysis explores the effects on the surface interaction models arising from the requirement that the shear mode properties are correctly accounted for.

The inelastic electron scattering measurements were carried out using a new multichannel detection electron energy loss spectrometer which has been described in recent publications[1-3]. The new instrument achieves 4-5 meV energy resolution and offers unique mechanical flexibility which permits both in-plane and out-of-plane scattering measurements over a wide range of scattering geometries and kinematical conditions.

Experimental results for Ag(110) along $\overline{\Gamma}-\overline{X}$ include a pair of even symmetry modes and an odd symmetry mode all of which exhibit conventional dispersion. The shear mode energy is the lowest, 3.5 meV at $\overline{X}$ followed by the even symmetry Rayleigh mode which appears to split near 1/2 $\overline{X}$ and which has mode energies of 5.6 meV and 6.0 meV at $\overline{X}$. This splitting results from contributions to inelastic scattering from surface and second layer vibrations. The upper even symmetry mode appears to have a maximum value at approximately 3/4 $\overline{X}$ (10 meV) and a slightly lower energy (9 meV) at $\overline{X}$. The phonon properties along $\overline{\Gamma}-\overline{Y}$ are similar with the exception that the lower even symmetry mode does not appear to split at $\overline{Y}$, and all mode energies at $\overline{Y}$ are lower: odd symmetry mode, 3.2 meV, lower even symmetry mode, 6.0 meV, upper even symmetry mode 7.5 meV, (at $\overline{Y}$) and maximum at 3/4 $\overline{Y}$ 9 meV.

The theoretical analysis of the surface modes of Ag(100) and Ag(110) is based on a lattice dynamical model for bulk Ag proposed by Black *et al.*[4](model Ag-III). The model incorporates angle bending forces to account for the violation of the Cauchy relation by Ag.

A fit to the observed surface modes described above shows that there is significant softening in the first neighbor force constants at the Ag(100) and Ag(110) surfaces. This softening is necessitated by the presence of (unexpectedly) low-lying odd symmetry shear modes. Thus the observation of these shear modes has led to a lattice dynamical model for the Ag(100) and Ag(110) surfaces which is significantly different from a model that would have been based on the even modes alone. This demonstrates the extreme importance of having available a *complete* set of surface modes (even *and* odd) for the development of realistic surface dynamical models.

This work was sponsored by AFOSR 90-0058, NSF DMR 88-16301, the Robert A. Welch Foundation, and the Joint Services Electronic Programs AFOSR-F49620-86-C-0045.

1. F. Hadjarab and J.L. Erskine, *J. Electron Spect. Rel. Phenom.* **36**, 227 (1985).
2. Eue-Jin Jeong and J.L. Erskine, *Rev. Sci. Instrum.* **60** (10), 3139 (1989).
3. A. Sellidj and J.L. Erskine, *Rev. Sci. Instrum.* **61** (1) 49 (1990).
4. J.E. Black, F.C. Shanes, and R.F. Wallis, *Surf. Sci.* **133**, 199 (1983).

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6.	SENIOR RESEARCH PERSONNEL	None
7.	JUNIOR RESEARCH PERSONNEL	J. Woods (Ph.D. 1986) A. Sellidj (Ph.D. 1989) E. Jeong (Ph.D. 1989) Y. Li (Ph.D. 1990) J. Yater Student
8.	PUBLICATIONS (Reprints Attached)	

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J. P. Woods, A. D. Kulkarni, J. L. Erskine and F. W. deWette, "Vibrational Properties of ß1H and ß1D on W(001): Electron Energy Loss Measurements and Lattice-dynamical Calculations", Phys. Rev. B36, 5848 (1987).

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J.L. Erskine, J.P. Woods, A.D. Kulkarni, and F.W. deWette, "Surface Vibrations on Clean and Hydrogen Saturated W(100)", J. of Electron Spectro. and Related Phenom. 44, 27 (1987).

B.-S. Fang, C.. . Ballentine, and J.L. Erskine, "Hydrogen Adsorption at Nb(100): Photoemission Evidence of Two-state Exchange Involving Subsurface States", Surface Science Letters 204, L713 (1988).

Eue-Jin Jeong and J.L. Erskine, "Multichannel Detection High Resolution Electron Energy Loss Spectrometer", Review of Scien. Instrum. 60, 3139 (1989).

A. Sellidj and J.L. Erskine, "Electron Energy Loss Spectroscopy Studies of Nitrogen Adsorption on W(100)", Surface Science 220, 253 (1989).

A. Sellidj and J.L. Erskine, "A Tandem Four-element Lens System for Inelastic Electron Scattering Studies", Rev. Sci. Inst. (in press).

J.L. Erskine, Eue-Jin Jeong, Joan Yater, Y. Chen, and S.Y. Tong, "Detection of Odd Symmetry Shear Modes at Metal Surfaces by Inelastic Electron Scattering: Experiment and Theory", (submitted to J. Vac. Sci. and Tech.,) (1989).

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"High Resolution Electron Energy Loss Spectroscopy Studies of the Interaction of H with Nb(100)", Y. Li, J. L. Erskine and A. Diebold, Bull. Am. Phys. Soc. 31, 272 (1986)

"High Resolution Electron Energy Loss Spectroscopy of Adsorbates at Metal Surfaces", J. L. Erskine, Joint Meeting of the Texas Section of the APS and AAPT; Abilene Christian University, Abilene, Texas, March 6-7, 1987.

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"Surface Vibrations on Clean and Hydrogen Saturated W(100)", J.L. Erskine, J.P. Woods, A.D. Kulkarni and F.W. deWette, Vibrations at Surfaces V, Eibsee Hotel, D-8104 Grainau-Eibsee, Fed. Rep. Germany, Sept. 6-10, 1987.

"Vibrational Spectroscopy Studies of Hydrogen at Metal Surfaces", J.L. Erskine, AFOSR Surface Chemistry Contractors Conference; Air Force Academy, Colorado Springs, Colorado, Sept. 16-18, 1987.

"Surface Vibrations on Clean and Hydrogen Covered Nb(110) Surfaces", Y. Li, A.D. Kulkarni, J.L. Erskine, and F.W. DeWette, March Meeting of the American Physical Society, New Orleans, Louisiana, March 21-25, 1988, Bull. Am. Phys. Soc. 33, 655 (1988).

"Electron Energy Loss Spectroscopy Study of N2 and H2 Chemisorption on W(100) at 105K", A. Sellidj and J.L. Erskine, March Meeting of the American Physical Society, New Orleans, Louisiana, March 21-25, 1988, Bull. Am. Phys. Soc. 33, 818 (1988).

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"UPS Study of Nitrogen Adsorption on W(100) at 135 K", A. Sellidj and J.L. Erskine, March Meeting of the American Physical Society, St. Louis, Missouri, March 20-24, 1989, Bull. Am. Phys. Soc. 34 (3) [1989].

"Inelastic Electron Scattering Studies of Surface Phonons", J.L. Erskine, Department of Physics, Indiana University, Bloomington, Indiana, April 7, 1989.

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"Inelastic Electron Scattering from Surfaces and Thin Epitaxial Layers", J.L. Erskine, Molecular Dynamics Workshop, Captive Island, Florida, Oct. 29-31, 1989.

"Detection of Odd-symmetry Shear Modes at Metal Surfaces by Inelastic Electron Scattering: Experiment and Theory", J.L. Erskine, Eue-Jin Jeong, Joan Yater, Y. Chen, and S.Y. Tong, 36th National Symposium of The American Vacuum Society, Boston, Massachusetts, Oct. 23-27, 1989.

9 ABSTRACT OF OBJECTIVES AND ACCOMPLISHMENTS

This research program utilizes inelastic electron scattering and other complementary spectroscopy probes of surfaces to investigate the structure, chemical properties and physical properties of surfaces. Research accomplishments of the program include a significant advancement in instrumentation, the first measurements of shear horizontal vibrational modes at crystal surfaces, the first detection of projected bulk phonon modes by surface electron scattering and elucidation of novel properties associated with hydrogen interaction at Nb surfaces.

The first observation of shear horizontal modes on Ni(100), Ag(100) and Ag(110) was made possible by the capability of our new instrument to detect out-of-plane scattering, combined with the improved sensitivity of the electron optics. Our new results including the shear modes constitute the first complete characterization of all surface vibrational modes at a single crystal surface. These data provide tests of selection rules that govern inelastic electron scattering and are presently being used in conjunction with lattice dynamical calculations to refine our understanding of interatomic potentials that bind crystals and govern thin film growth, and interface stability.

Inelastic electron scattering and angle resolved photoemission studies of the interaction of H with Nb have established the existence of a metastable subsurface binding site of hydrogen just below the surface. The location of the hydrogen site (tetrahedral) has been deduced based on vibrational data, and the novel thermal properties of the site occupation have been studied by photoemission and electron scattering. These studies have provided a detailed microscopic basis for explaining the novel uptake kinetics associated with the H/Nb system and have tested calculations of the ground state electronic properties of Nb and the H/Nb system.